Auramine 492-80-8 | DTXSID7043821

Model Performan	nce
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Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.42e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.38e-01

Confidence level: 5.24e-01

Nearest Neighbors from the Training Set

Image not found

Fipronil

Measured: 3.68e-06 Predicted: 8.03e-10

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Methyl salicylate

Measured: 5.27e-06 Predicted: 4.27e-03

Image not found

Mefenacet

Measured: 8.30e-08 Predicted: 1.64e-08

Image not found

Flumioxazin

Measured: 1.74e-07 Predicted: 9.24e-07

Image not found

Tetranitromethane Measured: 2.20e-06 Predicted: 1.23